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Maximum Zagreb index, minimum hyper-Wiener index and graph connectivity

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ABSTRACT

In this work we show that among all n-vertex graphs with edge or vertex connectivity k, the graph $G = K_k \vee (K_1 + K_{n-k-1})$, the join of K_k, the complete graph on k vertices, with the disjoint union of K_1 and K_{n-k-1}, is the unique graph with maximum sum of squares of vertex degrees. This graph is also the unique n-vertex graph with edge or vertex connectivity k whose hyper-Wiener index is minimum.

1. Introduction

Throughout this work we consider simple graphs, the graphs without loops and multiple edges. Our notation is standard and is taken from [1]. Let $G = (V, E)$ be a graph with vertex set $V = V(G)$ and edge set $E = E(G)$. We denote by $d(x, y)$, $N(x)$ and $\deg(x)$, the distance between vertices x and y, vertices at distance 1 from vertex x and the degree of x, respectively.

A graphical invariant is a number related to a graph which is structurally invariant, that is to say it is fixed under graph automorphisms. In chemistry and for molecular graphs, these invariant numbers are known as the topological indices. The Wiener index, denoted by W, is perhaps the most studied topological index from application and theoretical viewpoints. This index is defined as the sum of all distances between vertices of a graph [2]. Randić [3] introduced an extension of the Wiener index for trees, and this has come to be known as the hyper-Wiener index, denoted by WW. Klein et al. [4] generalized this extension to cyclic structures as

$$WW(G) = \frac{1}{2} \sum_{\{u,v\} \subseteq V(G)} (d(u, v) + d(u, v)^2).$$

The graph invariant hyper-Wiener index is also a distance based graph invariant. One of the oldest graph invariants is the first Zagreb index, which was introduced by Gutman and Trinajstić [5], and is denoted by M_1. It is defined as the sum of squares of vertex degrees of the graph,

$$M_1(G) = \sum_{v \in V(G)} \deg(v)^2.$$

The hyper-Wiener and Zagreb indices are widely studied. It is a primary result that among all trees with a fixed number of vertices, a star has the minimum Wiener and hyper-Wiener indices and a path has the maximum Wiener and hyper-Wiener

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indices. The graphs with a fixed number of edges and vertices, with smallest Zagreb index are completely characterized in [6]. For more details and results see [7–9].

Recall that if G is a connected graph on n vertices which is not a complete graph, then the vertex connectivity (or simply the connectivity) of G is equal to k if all subgraphs of G obtained by deleting from G fewer than k vertices are connected, and there exists a disconnected subgraph of G obtained by deleting exactly k vertices from G. In this case we say that G is k-connected. The vertex connectivity of the complete graph K_n on n vertices is defined as $n-1$. If k is the connectivity of G, then $1 \le k \le n-1$, with $k = n-1$ if and only if $G = K_n$. Similarly, if G is a connected graph on n vertices, then the edge connectivity of G is equal to k if all subgraphs of G obtained by deleting from G fewer than k edges are connected, and there exists a disconnected subgraph of G obtained by deleting exactly k edges from G. If k is the edge connectivity of G, then $1 \le k \le n-1$, with $k = n-1$ if and only if $G = K_n$.

Recently Gutman and Zhang [10] proved that among all n-vertex graphs with (vertex or edge) connectivity k the graph $K_k \vee (K_1 + K_{n-k-1})$, which is the graph obtained by connecting all vertices of the complete graph K_k with all vertices of the graph whose two components are K_1 and K_{n-k-1}, that is the join of the graph K_k with the disjoint union of K_1 and K_{n-k-1}, is the unique graph having minimum Wiener index.

In this work we consider an analogous problem for Zagreb and hyper-Wiener indices. We show that among all n-vertex graphs with (vertex or edge) connectivity k, $K_k \vee (K_1 + K_{n-k-1})$ is the unique graph with maximum Zagreb index. We also show that this graph among all n-vertex graphs with (vertex or edge) connectivity k is the unique graph with minimum hyper-Wiener index.

2. Maximum Zagreb index and connectivity

Adding any new edge to a fixed non-complete graph will increase the degree of two vertices of it and so increases properly its Zagreb index. So obviously the complete graph on n vertices is the unique n-vertex graph whose Zagreb index is maximum. But the vertex and edge connectivity of K_n is $n-1$. In the general case when the connectivity is less than $n-1$, the graph whose Zagreb index is maximum is also unique but the proof of this fact is not straightforward. In the following theorems we follow the proofs given in [10].

Theorem 1. *Let H be an n-vertex graph, $n \ge 2$, with vertex connectivity k. Then $M_1(H) \le n(n-1)^2 + (n-k-1)(4-3n-k)$, and the equality holds if and only if $H \cong K_k \vee (K_1 + K_{n-k-1})$.*

Proof. Let G be a graph such that among all n-vertex graphs with vertex connectivity, k has maximum Zagreb index. By hypothesis there exists a k-element set $S \subseteq V(G)$ such that $G - S$ is disconnected. Let $G_1, G_2, \ldots, G_r$ be connected components of $G - S$. If $r > 2$, then adding an edge between G_1 and G_2 will preserve the connectivity of G but increase the Zagreb index and this contradicts the maximality of G. So $r = 2$ and $G - S$ has exactly two connected components G_1 and G_2. By a similar argument we can see that G_1, G_2 and the induced subgraph $G[S]$ should be complete graphs. Also all vertices in S are adjacent with all vertices in G_1 and G_2. Let $n_1 = |V(G_1)|$ and $n_2 = |V(G_2)|$ and so $n = n_1 + n_2 + k$. All vertices of S have the same degree $n_1 + n_2 + (k-1) = n-1$. Also if $x \in V(G_1)$ and $y \in V(G_2)$, then $\deg(x) = k + (n_1 - 1)$ and $\deg(y) = k + (n_2 - 1)$. It follows that

$$\begin{aligned} M_1(G) &= n_1((n_1-1)+k)^2 + n_2((n_2-1)+k)^2 + k(n-1)^2 \\ &= n_1(n-n_2-1)^2 + n_2(n-n_1-1)^2 + k(n-1)^2 \\ &= n_1(n-1)^2 - 2n_1n_2(n-1) + n_1n_2^2 + n_2(n-1)^2 - 2n_1n_2(n-1) + n_2n_1^2 + k(n-1)^2 \\ &= (n_1+n_2+k)(n-1)^2 - 4n_1n_2(n-1) + n_1n_2^2 + n_2n_1^2 \\ &= n(n-1)^2 + n_1n_2(n_1+n_2-4(n-1)) \\ &= n(n-1)^2 + n_1n_2(4-3n-k). \end{aligned}$$

Now since n, the order of G, is a fixed number and $(4-3n-k) < 0$, the maximality of $M_1(G)$ implies that the product n_1n_2 should be minimum. Now since $n_1 + n_2 = n - k$ and $1 \le n_1, n_2 \le n-1-k$, we must have $\{n_1, n_2\} = \{1, n-1-k\}$. Therefore $M_1(G) = (n-1)^2 + (n-k-1)(4-3n-k)$ and $G \cong K_k \vee (K_1 + K_{n-k-1})$. Now since, by direct computation,

$$M_1(G) = n(n-1)^2 + (n-k-1)(4-3n-k)$$

the proof is complete. ■

To prove a similar result for graphs with edge connectivity k, we need the following lemma on bipartite graphs with a fixed number of edges.

Lemma 2. *If H is a bipartite graph with k edges and without isolated vertices, then $M_1(H) \le k^2 + k$ and the equality holds if and only if $H \cong S_{k+1}$, the star graph on $k+1$ vertices.*

Proof. Let G be a k-edge bipartite graph with bipartition (S, T) whose Zagreb index is maximum among all bipartite graphs with exactly k edges. For readability of the proof we divide the proof into steps.

Claim 1. *Each part of G has a vertex which is adjacent to all vertices in the other part.*

Proof. Let $x \in S$ be a vertex whose degree is maximum among vertices in S and let $\Delta_1 = \deg(x)$. If there exists a vertex $y \in S$ which is adjacent to a vertex $t \in T$ but x is not adjacent to t, then by replacing the edge yt by edge xt we obtain a new bipartite graph G' with the same number of edges. But in this case we have

$$M_1(G') - M_1(G) = [(\Delta_1 + 1)^2 + (\deg(y) - 1)^2] - [\Delta_1^2 + \deg(y)^2] = 2 + 2(\Delta_1 - \deg(y)) > 0,$$

which contradicts the maximality of G. Thus x is adjacent to all vertices in T. The argument for T is similar.

Claim 2. *If all vertices of a part have the same degree, then all vertices of the other part also have the same degree.*

Proof. Assume that all vertices in S have the same degree Δ_1 and let $\Delta_2 = \mathrm{Max}\{\deg(t) | t \in T\}$. By Claim 1, we have $|S| = \Delta_2$ and $|T| = \Delta_1$ and so

$$\Delta_2\Delta_1 = \sum_{s\in S} \deg(s) = |E(G)| = k = \sum_{t\in T} \deg(t) \le \sum_{t\in T} \Delta_2 = \Delta_1\Delta_2,$$

which implies that $\deg(t) = \Delta_2$ for each $t \in T$.

Claim 3. *If all vertices in each part have the same degree, then $G \cong S_{k+1}$.*

Proof. With the notation of Claim 2 we have $k = \Delta_1\Delta_2$ and

$$M_1(G) = \sum_{s\in S} \deg(s)^2 + \sum_{t\in T} \deg(t)^2 = \Delta_2\Delta_1^2 + \Delta_1\Delta_2^2 = k\left(\Delta_1 + \frac{k}{\Delta_1}\right), \quad 1 \le \Delta_1 \le k.$$

Let $f(x) = kx + \frac{k^2}{x}$, $1 \le x \le k$. Solving $f'(x) = 0$ yields $x = \pm\sqrt{k}$, and since

$$f(\sqrt{k}) = k\sqrt{k} + \frac{k^2}{\sqrt{k}}, \qquad f(-\sqrt{k}) = -k\sqrt{k} + \frac{k^2}{-\sqrt{k}}, \qquad f(1) = k^2 + k = f(k),$$

we have $\mathrm{Max}\{f(x) \mid 1 \le x \le k\} = k^2 + k$. Now maximality of $M_1(G)$ implies that $\Delta_1 = k$ and $\Delta_2 = 1$, say, and this forces that the graph G is the star S_{k+1}.

Note that without loss of generality we can assume $\Delta_2 \le \Delta_1$. So in what follows we assume that Δ_1 is equal to or greater than Δ_2.

Claim 4. *All vertices of the S part have the same degree.*

Proof. Suppose, on the contrary, that there exists a vertex $x \in S$ whose degree is less than Δ_1, the maximum degree among all vertices in S. Let $j = \deg(x)$, $j \ge 1$, and $N(x) = \{t_1, t_2, \dots, t_j\}$. By removing j edges which are incident to x and adding j new vertices to the T part and connecting them to a vertex of degree Δ_1 in S by j new edges, we obtain a new bipartite graph G' with exactly k edges. An easy calculation yields

$$\begin{aligned} M_1(G') - M_1(G) &= \left[(\Delta_1 + j)^2 + (\deg(t_1) - 1)^2 + \cdots + (\deg(t_j) - 1)^2 + j \times 1^2\right] \\ &\quad - \left[\Delta_1^2 + j^2 + \deg(t_1)^2 + \cdots + \deg(t_j)^2\right] \\ &= 2j\Delta_1 + 2j - 2(\deg(t_1) + \cdots + \deg(t_j)) \\ &= 2j + 2((\Delta_1 - \deg(t_1)) + \cdots + (\Delta_1 - \deg(t_j))) > 0, \end{aligned}$$

which contradicts the maximality of $M_1(G)$. So all vertices in S have the same degree Δ_1.

Now since Claim 4 is valid, Claim 2 implies that all vertices in the part T also have the same degree Δ_2 and this using Claim 3 forces that the graph G is the star S_{k+1}, and this completes the proof. ■

Now we are ready to prove the following theorem which is also our main theorem of this section.

Theorem 3. *Let H be a graph of order n, $n \ge 2$, and edge connectivity k; then $M_1(H) \le (n-1)(n-2)^2 + k(k + 2n - 3)$, and the equality holds if and only if $H \cong K_k \vee (K_1 + K_{n-k-1})$.*

Proof. Let G be a graph such that among all n-vertex graphs with edge connectivity k it has maximum Zagreb index. By hypothesis there exists an edge cut $M \subseteq E(G)$ of size k. By an argument similar to that in Theorem 1 and by maximality of $M_1(G)$ we can see that $G - M$ is disconnected with exactly two connected components G_1 and G_2 which are also complete graphs as induced subgraphs. Denote the set of the end-points of the edges of M in G_1 by S and the set of the end-points of the edges of M in G_2 by T. So if we let $n_1 = |V(G_1)|$ and $n_2 = |V(G_2)|$, then $n = n_1 + n_2$ and

$$\begin{aligned} M_1(G) &= \sum_{x\in V(G_1)} \deg(x)^2 + \sum_{y\in V(G_2)} \deg(y)^2 \\ &= \left[n_1(n_1-1)^2 + 2(n_1-1)\sum_{s\in S}\deg(s) + \sum_{s\in S}\deg(s)^2 \right] \\ &\quad + \left[n_2(n_2-1)^2 + 2(n_2-1)\sum_{t\in T}\deg(t) + \sum_{t\in T}\deg(t)^2 \right] \\ &= n_1(n_1-1)^2 + n_2(n_2-1)^2 + 2k(n-2) + \sum_{s\in S}\deg(s)^2 + \sum_{t\in T}\deg(t)^2, \end{aligned}$$

where $\deg(s)$ and $\deg(t)$ are computed in the induced subgraph of G obtained from the edge set M. Now it is easy (in the above formula take k edges incident to the unique vertex of K_1 as the edge cut M) to check that

$$\begin{aligned} M_1(K_k \vee (K_1 + K_{n-k-1})) &= (n-1)(n-2)^2 + 2k(n-2) + k^2 + k \\ &= (n-1)^2 n + (n-1)(4-3n) + 2k(n-2) + k^2 + k. \end{aligned}$$

On the other hand we have

$$\begin{aligned} n_1(n_1-1)^2 + n_2(n_2-1)^2 &= n_1((n-n_2)-1)^2 + n_2((n-n_1)-1)^2 \\ &= n_1[(n-1)^2 - 2(n-1)n_2 + n_2^2] + n_2[(n-1)^2 - 2(n-1)n_1 + n_1^2] \\ &= (n-1)^2(n_1+n_2) - 4(n_1-1)n_1n_2 + n_1n_2^2 + n_2n_1^2 \\ &= (n-1)^2 n + n_1n_2(4-3n). \end{aligned}$$

Since $4 - 3n < 0$ and $1 \le n_1, n_2 \le n-1$ we have

$$n_1(n_1-1)^2 + n_2(n_2-1)^2 \le (n-1)^2 n + (n-1)(4-3n)$$

with equality if and only if $\{n_1, n_2\} = \{1, n-1\}$. Now since the subgraph induced by the edge set M is a bipartite graph with exactly k edges, by Lemma 2 we obtain $\sum_{s\in S}\deg(s)^2 + \sum_{t\in T}\deg(t)^2 \le k^2 + k$. But by assumption, $M_1(G)$ is maximum and since $K_k \vee (K_1 + K_{n-k-1})$ is an n-vertex graph with edge connectivity k, we must have

$$n_1(n_1-1)^2 + n_2(n_2-1)^2 = (n-1)^2 n + (n-1)(4-3n)$$

and

$$\sum_{s\in S}\deg(s)^2 + \sum_{t\in T}\deg(t)^2 = k^2 + k$$

and these imply that $\{n_1, n_2\} = \{1, n-1\}$, that is the graph G is isomorphic to $K_k \vee (K_1 + K_{n-k-1})$. This completes the proof. ∎

3. Minimum hyper-Wiener index and connectivity

In this section we investigate similar results but for minimality of the hyper-Wiener index for graphs with a fixed number of vertices and fixed vertex or edge connectivity.

Theorem 4. *For every n-vertex graph H with connectivity k, $1 \le k \le n-1$, we have*

$$WW(H) \ge \binom{n}{2} + 2(n-k-1).$$

Equality holds if and only if $H \cong K_k \vee (K_1 + K_{n-k-1})$.

Proof. Let G be a graph such that among all n-vertex graphs with connectivity k it has minimum hyper-Wiener index. Let $S \subseteq V(G)$ be a separating set with $|S| = k$, and $G_1, G_2, \ldots, G_r$ be the connected components of $G - S$. Note that $r = 2$; otherwise by adding a new edge between G_1 and G_2, the connectivity of G will remain k as before, but the hyper-Wiener index will properly decrease and this contradicts the choice of G. Therefore $r = 2$ and $G - S$ has exactly two connected components G_1 and G_2. In a similar way we obtain that G_1, G_2 and the induced subgraph $G[S]$ are complete graphs. Also all vertices in S are adjacent to all vertices in $V(G) - S$. Let $n_1 = |V(G_1)|$ and $n_2 = |V(G_2)|$. Then $n = n_1 + n_2 + k$. So by an easy computation we have

$$\begin{aligned} WW(G) &= \frac{1}{2}\left[\binom{n_1}{2} + \binom{n_2}{2} + \binom{k}{2} + k(n_1+n_2) + 2n_1n_2\right] + \frac{1}{2}\left[\binom{n_1}{2} + \binom{n_2}{2} + \binom{k}{2} + k(n_1+n_2) + 4n_1n_2\right] \\ &= \frac{1}{2}(n_1^2 + n_2^2 + 2n_1n_2) - \frac{1}{2}(n_1+n_2+k) + \frac{1}{2}k^2 + k(n-k) + 2n_1n_2 \\ &= \frac{1}{2}((n-k)^2 + k^2 + 2k(n-k)) - \frac{1}{2}n + 2n_1n_2 \\ &= \binom{n}{2} + 2n_1n_2. \end{aligned}$$

In order to minimize $WW(G)$ it is necessary and sufficient to minimize the product of n_1 and n_2. Now since $n_1 + n_2 = n - k$ and $1 \le n_1, n_2 \le n - 1 - k$, we should have $\{n_1, n_2\} = \{1, n - 1 - k\}$. Therefore $G \cong K_k \vee (K_1 + K_{n-k-1})$. Since, by direct calculation, we have

$$WW(G) = \binom{n}{2} + 2(n-k-1)$$

the proof is complete. ■

In the edge connectivity case the argument is similar but it needs some more careful computations.

Theorem 5. *Let H be a graph of order n and edge connectivity k, $1 \le k \le n-1$. Then $WW(H) \ge \binom{n}{2} + 2(n-k-1)$, and the equality holds if and only if $H \cong K_k \vee (K_1 + K_{n-k-1})$.*

Proof. Let G be a graph such that among all n-vertex graphs with edge connectivity k it has minimum hyper-Wiener index. Let $M \subseteq E(G)$ be an edge cut of order k, and G_1, G_2 be connected components of $G - M$. As in the proof of Theorem 4, the subgraphs G_1 and G_2 must be complete graphs. Again let $n_1 = |V(G_1)|$ and $n_2 = |V(G_2)|$, so $n = n_1 + n_2$. Also suppose that the end-point vertices of the edges of M in G_1 and G_2 are S_1 and S_2, respectively. Let $t_1 = |V(G_1 - S_1)|$ and $t_2 = |V(G_2 - S_2)|$. Then there are t_1t_2 pairs of vertices with distance 3, $|E(G)|$ pairs of vertices with distance 1 and $\binom{n}{2} - t_1t_2 - |E(G)|$ pairs of vertices with distance 2. Now by an easy calculation we see that

$$\begin{aligned} WW(G) &= \frac{1}{2}\left[2|E(G)| + 6\left(\binom{n}{2} - t_1t_2 - |E(G)|\right) + 12t_1t_2\right] \\ &= 3\binom{n}{2} + 3t_1t_2 - 2|E(G)| \\ &= \frac{3}{2}n(n-1) + 3t_1t_2 - 2\left[\frac{1}{2}n_1(n_1-1) + \frac{1}{2}n_2(n_2-1) + k\right] \\ &= \frac{3}{2}n(n-1) - 2k + 3t_1t_2 - n_1((n-n_2)-1) - n_2((n-n_1)-1) \\ &= \frac{1}{2}n(n-1) - 2k + 3t_1t_2 + 2n_1n_2. \end{aligned}$$

Since $\frac{1}{2}n(n-1) - 2k$ is a fixed number, minimality of $WW(G)$ implies that $3t_1t_2 + 2n_1n_2$ is minimum. Now since $1 \le n_1, n_2 \le n-1$, $n_1 + n_2 = n$ and $0 \le t_i < n_i$, for $i = 1, 2$, we should have $\{n_1, n_2\} = \{1, n-1\}$ and so $n_1n_2 = n-1$ and $t_1t_2 = 0$. Without loss of generality, suppose that $n_1 = 1$ and so $n_2 = n-1$. This implies that the single vertex of the component G_1 is adjacent through k edges to the vertices in S_2 and so $|S_2| = k$ and $t_2 = (n-1) - k$, which implies that G is isomorphic to the graph $K_k \vee (K_1 + K_{n-k-1})$. ■

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